(E)-4-Tridecen-2-yl acetate

Inchi: InChI=1S/C15H28O2/c1-4-5-6-7-8-9-10-11-12-13-14(2)17-15(3)16/h11-12,14H,4-10,13H
InchiKey: KHLRNGQOCNTDNQ-VAWYXSNFSA-N
Formula: C15H28O2
SMILES: CCCCCCCCC=CCC(C)OC(C)=O
Mol. weight [g/mol]: 240.38

Physical Properties

Property code	Value	Unit	Source
gf	-80.72	kJ/mol	Joback Method
hf	-485.79	kJ/mol	Joback Method
hfus	34.07	kJ/mol	Joback Method
hvap	57.71	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.635		Crippen Method
mcvol	225.350	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
rinpol	1616.00		NIST Webbook
ripol	1884.00		NIST Webbook
ripol	1884.00		NIST Webbook
tb	622.61	K	Joback Method
tc	798.28	K	Joback Method
tf	310.89	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.96	J/mol×K	622.61	Joback Method
cpg	679.98	J/mol×K	769.00	Joback Method
cpg	665.65	J/mol×K	739.72	Joback Method
cpg	650.60	J/mol×K	710.44	Joback Method
cpg	634.82	J/mol×K	681.17	Joback Method
cpg	618.28	J/mol×K	651.89	Joback Method
cpg	693.62	J/mol×K	798.28	Joback Method

dvisc	0.0001094	Pa×s	622.61	Joback Method
dvisc	0.0001488	Pa×s	570.66	Joback Method
dvisc	0.0002154	Pa×s	518.70	Joback Method
dvisc	0.0003383	Pa×s	466.75	Joback Method
dvisc	0.0005952	Pa×s	414.80	Joback Method
dvisc	0.0012311	Pa×s	362.84	Joback Method
dvisc	0.0032461	Pa×s	310.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R203488&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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